Christian SchrÃ¶der

List of Publications by Year
in descending order

92	3,496	126708	149479
papers	citations	33 h-index	56 g-index

93	93	93	2886
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Molecular Dynamics Simulations of Ionic Liquids and Electrolytes Using Polarizable Force Fields. Chemical Reviews, 2019, 119, 7940-7995.	23.0	386
2	Comparing reduced partial charge models with polarizable simulations of ionic liquids. Physical Chemistry Chemical Physics, 2012, 14, 3089.	1.3	229
3	On the collective network of ionic liquid/water mixtures. I. Orientational structure. Journal of Chemical Physics, 2007, 127, 234503.	1.2	120
4	On the computation and contribution of conductivity in molecular ionic liquids. Journal of Chemical Physics, 2008, 128, 134501.	1.2	117
5	Proteins in Ionic Liquids: Current Status of Experiments and Simulations. Topics in Current Chemistry, 2017, 375, 25.	3.0	117
6	Surface-active ionic liquids: A review. Journal of Molecular Liquids, 2022, 347, 118160.	2.3	108
7	Simulation studies of ionic liquids: Orientational correlations and static dielectric properties. Journal of Chemical Physics, 2006, 125, 244506.	1.2	99
8	Simulating polarizable molecular ionic liquids with Drude oscillators. Journal of Chemical Physics, 2010, 133, 154511.	1.2	98
9	On the collective network of ionic liquid/water mixtures. II. Decomposition and interpretation of dielectric spectra. Journal of Chemical Physics, 2008, 129, 184501.	1.2	95
10	Collective rotational dynamics in ionic liquids: A computational and experimental study of 1-butyl-3-methyl-imidazolium tetrafluoroborate. Journal of Chemical Physics, 2007, 126, 084511.	1.2	93
11	Intramolecular vibrational energy redistribution in bridged azulene-anthracene compounds: Ballistic energy transport through molecular chains. Journal of Chemical Physics, 2004, 121, 1754-1764.	1.2	89
12	Micellar catalysis in aqueousâ€“ionic liquid systems. Chemical Communications, 2012, 48, 5013.	2.2	79
13	Simulation studies of the protein-water interface. I. Properties at the molecular resolution. Journal of Chemical Physics, 2006, 124, 234907.	1.2	75
14	Surface-active ionic liquids in micellar catalysis: impact of anion selection on reaction rates in nucleophilic substitutions. Physical Chemistry Chemical Physics, 2016, 18, 13375-13384.	1.3	68
15	Computational studies of ionic liquids: Size does matter and time too. Journal of Chemical Physics, 2012, 137, 094501.	1.2	64
16	Polarisabilities of alkylimidazolium ionic liquids. Physical Chemistry Chemical Physics, 2013, 15, 2703.	1.3	64
17	Collective translational motions and cage relaxations in molecular ionic liquids. Journal of Chemical Physics, 2011, 135, 024502.	1.2	60
18	On the dielectric conductivity of molecular ionic liquids. Journal of Chemical Physics, 2009, 131, 114504.	1.2	58

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19	Alchemical free energy calculations and multiple conformational substates. Journal of Chemical Physics, 2005, 122, 084109.	1.2	56
20	Using fit functions in computational dielectric spectroscopy. Journal of Chemical Physics, 2010, 132, 244109.	1.2	54
21	On the collective network of ionic liquid/water mixtures. III. Structural analysis of ionic liquids on the basis of Voronoi decomposition. Journal of Chemical Physics, 2009, 130, 194503.	1.2	50
22	Impact of anisotropy on the structure and dynamics of ionic liquids: A computational study of 1-butyl-3-methyl-imidazolium trifluoroacetate. Journal of Chemical Physics, 2007, 127, 044505.	1.2	49
23	The influence of electrostatic forces on the structure and dynamics of molecular ionic liquids. Journal of Chemical Physics, 2008, 128, 224503.	1.2	49
24	The influence of polarizability on the dielectric spectrum of the ionic liquid 1-ethyl-3-methylimidazolium triflate. Physical Chemistry Chemical Physics, 2011, 13, 12240.	1.3	47
25	Hydrated Ionic Liquids with and without Solute: The Influence of Water Content and Protein Solutes. Journal of Chemical Theory and Computation, 2012, 8, 3911-3928.	2.3	47
26	Dielectric and Terahertz Spectroscopy of Polarizable and Nonpolarizable Water Models: A Comparative Study. Journal of Physical Chemistry A, 2015, 119, 1539-1547.	1.1	47
27	Quantum mechanical determination of atomic polarizabilities of ionic liquids. Physical Chemistry Chemical Physics, 2018, 20, 10992-10996.	1.3	47
28	Solvation studies of a zinc finger protein in hydrated ionic liquids. Physical Chemistry Chemical Physics, 2011, 13, 6955.	1.3	45
29	Exploring ionic liquidâ€“biomass interactions: towards the improved isolation of shikimic acid from star anise pods. RSC Advances, 2013, 3, 26010.	1.7	43
30	Simulation studies of the protein-water interface. II. Properties at the mesoscopic resolution. Journal of Chemical Physics, 2006, 124, 234908.	1.2	39
31	Additive polarizabilities in ionic liquids. Physical Chemistry Chemical Physics, 2016, 18, 1665-1670.	1.3	37
32	Comparing induced point-dipoles and Drude oscillators. Physical Chemistry Chemical Physics, 2015, 17, 14297-14306.	1.3	36
33	Intramolecular vibrational redistribution and energy relaxation in solution: A molecular dynamics approachPresented at the annual meeting of the Deutsche Bunsen-Gesellschaft fÃ¼r Physikalische Chemie, Stuttgart, May 24â€“26, 2001.. Physical Chemistry Chemical Physics, 2002, 4, 271-278.	1.3	35
34	Relaxation of Voronoi shells in hydrated molecular ionic liquids. Journal of Chemical Physics, 2009, 131, 174509.	1.2	33
35	Polarization effects on the solvation dynamics of coumarin C153 in ionic liquids: Components and their cross-correlations. Journal of Chemical Physics, 2013, 138, 204504.	1.2	30
36	Basic chiral ionic liquids: A novel strategy for acid-free organocatalysis. Catalysis Today, 2013, 200, 80-86.	2.2	29

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37	Pair dynamics and the intermolecular nuclear Overhauser effect (NOE) in liquids analysed by simulation and model theories: Application to an ionic liquid. Journal of Chemical Physics, 2014, 140, 184503.	1.2	29
38	Thioglycolate-based task-specific ionic liquids: Metal extraction abilities vs acute algal toxicity. Journal of Hazardous Materials, 2017, 340, 113-119.	6.5	29
39	Molecular dynamics analysis of the effect of electronic polarization on the structure and single-particle dynamics of mixtures of ionic liquids and lithium salts. Journal of Chemical Physics, 2016, 145, 204507.	1.2	28
40	Molecular Dynamics Simulation of Heat Conduction through a Molecular Chain. Journal of Physical Chemistry A, 2009, 113, 14039-14051.	1.1	24
41	Communication: Solvation and dielectric response in ionic liquidsâ€"Conductivity extension of the continuum model. Journal of Chemical Physics, 2013, 138, 111102.	1.2	22
42	Solvation dynamics in polar solvents and imidazolium ionic liquids: failure of linear response approximations. Physical Chemistry Chemical Physics, 2018, 20, 5246-5255.	1.3	22
43	Toward Prediction of Electrostatic Parameters for Force Fields That Explicitly Treat Electronic Polarization. Journal of Chemical Theory and Computation, 2019, 15, 2460-2469.	2.3	21
44	Understanding the Nature of Nuclear Magnetic Resonance Relaxation by Means of Fast-Field-Cycling Relaxometry and Molecular Dynamics Simulationsâ€"The Validity of Relaxation Models. Journal of Physical Chemistry Letters, 2020, 11, 2165-2170.	2.1	21
45	The physical significance of the Kamletâ€"TaftÏ€* parameter of ionic liquids. Physical Chemistry Chemical Physics, 2021, 23, 1616-1626.	1.3	21
46	Amino alcohol-derived chiral ionic liquids: structural investigations toward chiral recognition. Tetrahedron: Asymmetry, 2015, 26, 1069-1082.	1.8	20
47	Evaluating excited state atomic polarizabilities of chromophores. Physical Chemistry Chemical Physics, 2018, 20, 8554-8563.	1.3	20
48	Dielectric spectra of ionic liquids and their conversion to solvation dynamics: a detailed computational analysis of polarizable systems. Physical Chemistry Chemical Physics, 2014, 16, 10999-11009.	1.3	19
49	Langevin behavior of the dielectric decrement in ionic liquid water mixtures. Physical Chemistry Chemical Physics, 2018, 20, 15106-15117.	1.3	19
50	The effect of Thole functions on the simulation of ionic liquids with point induced dipoles at various densities. Journal of Chemical Physics, 2013, 138, 204119.	1.2	18
51	Computational analysis of the solvation of coffee ingredients in aqueous ionic liquid mixtures. RSC Advances, 2017, 7, 3495-3504.	1.7	18
52	A shell-resolved analysis of preferential solvation of coffee ingredients in aqueous mixtures of the ionic liquid 1-ethyl-3-methylimidazolium acetate. Journal of Chemical Physics, 2018, 148, 193819.	1.2	17
53	Ion-Tagged Chiral Ligands for Asymmetric Transfer Hydrogenations in Aqueous Medium. ACS Sustainable Chemistry and Engineering, 2019, 7, 3414-3423.	3.2	17
54	Polarizable MD simulations of ionic liquids: How does additional charge transfer change the dynamics?. Physical Chemistry Chemical Physics, 2020, 22, 467-477.	1.3	17

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55	The small impact of various partial charge distributions in ground and excited state on the computational Stokes shift of 1-methyl-6-oxyquinolinium betaine in diverse water models. Journal of Chemical Physics, 2016, 145, 164506.	1.2	16
56	On the validity of linear response approximations regarding the solvation dynamics of polyatomic solutes. Physical Chemistry Chemical Physics, 2017, 19, 10940-10950.	1.3	16
57	Intrinsic Structure of the Interface of Partially Miscible Fluids: An Application to Ionic Liquids. Journal of Physical Chemistry C, 2015, 119, 28448-28461.	1.5	15
58	Selective Hydrogenation of Aldehydes Using a Wellâ€Defined Fe(II) PNP Pincer Complex in Biphasic Medium. ChemCatChem, 2018, 10, 4386-4394.	1.8	15
59	Proteins in Ionic Liquids: Current Status of Experiments and Simulations. Topics in Current Chemistry Collections, 2017, , 127-152.	0.2	15
60	Computational solvation analysis of biomolecules in aqueous ionic liquid mixtures. Biophysical Reviews, 2018, 10, 825-840.	1.5	14
61	Additive polarizabilities of halides in ionic liquids and organic solvents. Journal of Chemical Physics, 2018, 149, 044302.	1.2	14
62	Comparison between ab initio and polarizable molecular dynamics simulations of 1-butyl-3-methylimidazolium tetrafluoroborate and chloride in water. Journal of Molecular Liquids, 2021, 337, 116521.	2.3	14
63	On the collective network of ionic liquid/water mixtures. IV. Kinetic and rotational depolarization. Journal of Chemical Physics, 2014, 140, 204505.	1.2	13
64	Solvation dynamics: improved reproduction of the time-dependent Stokes shift with polarizable empirical force field chromophore models. Physical Chemistry Chemical Physics, 2019, 21, 17703-17710.	1.3	12
65	Polarizable molecular dynamics simulations of ionic liquids: Influence of temperature control. Journal of Chemical Physics, 2020, 152, 094105.	1.2	12
66	Orientational Alignment of Amyloidogenic Proteins in Pre-Aggregated Solutions. Physical Review Letters, 2015, 114, 128101.	2.9	11
67	Solvation of anthraquinone and TEMPO redox-active species in acetonitrile using a polarizable force field. Journal of Chemical Physics, 2021, 155, 074504.	1.2	11
68	Computational solvation dynamics of oxyquinolinium betaine linked to trehalose. Journal of Chemical Physics, 2016, 145, 164507.	1.2	10
69	Effect of a Tertiary Butyl Group on Polar Solvation Dynamics in Aqueous Solution: A Computational Approach. Journal of Physical Chemistry B, 2017, 121, 9639-9646.	1.2	10
70	Molecular dynamics simulation of aqueous 1â€‘dodecylâ€3â€‘methylimidazolium chloride: Emerging micelles. Journal of Molecular Liquids, 2018, 272, 766-777.	2.3	10
71	Surface-Active Ionic Liquids in Catalytic Water Splitting. Australian Journal of Chemistry, 2019, 72, 34.	0.5	10
72	Computational spectroscopy of trehalose, sucrose, maltose, and glucose: A comprehensive study of TDSS, NQR, NOE, and DRS. Journal of Chemical Physics, 2019, 150, 175102.	1.2	10

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73	Computational analysis of conductivity contributions in an ionic liquid mixture of 1-ethyl-3-methylimidazolium dicyanamide and tetrafluoroborate. Journal of Molecular Liquids, 2019, 288, 110993.	2.3	9
74	Non-additive electronic polarizabilities of ionic liquids: Charge delocalization effects. Journal of Molecular Liquids, 2022, 346, 117099.	2.3	9
75	ForConX: A forcefield conversion tool based on XML. Journal of Computational Chemistry, 2017, 38, 629-638.	1.5	8
76	Polarizability in ionic liquid simulations causes hidden breakdown of linear response theory. Physical Chemistry Chemical Physics, 2019, 21, 1023-1028.	1.3	8
77	Emulating proton transfer reactions in the pseudo-protic ionic liquid 1-methylimidazolium acetate. Physical Chemistry Chemical Physics, 2022, 24, 9277-9285.	1.3	8
78	The Intermolecular NOE Depends on Isotope Selection: Short Range vs Long Range Behavior. Journal of Physical Chemistry Letters, 2021, 12, 8658-8663.	2.1	6
79	Changes in protein hydration dynamics by encapsulation or crowding of ubiquitin: strong correlation between time-dependent Stokes shift and intermolecular nuclear Overhauser effect. RSC Advances, 2019, 9, 36982-36993.	1.7	5
80	Recent Developments in Polarizable Molecular Dynamics Simulations of Electrolyte Solutions. Journal of Computational Biophysics and Chemistry, 2022, 21, 415-429.	1.0	5
81	Charge delocalization and hyperpolarizability in ionic liquids. Journal of Molecular Liquids, 2022, 349, 118153.	2.3	5
82	Polarizable molecular dynamics simulations on the conductivity of pure 1-methylimidazolium acetate systems. Physical Chemistry Chemical Physics, 2022, 24, 15245-15254.	1.3	5
83	Quantum Yields for the Photodissociation of Iodine in Compressed Liquids and Supercritical Fluids. Zeitschrift Fur Physikalische Chemie, 2001, 215, .	1.4	4
84	Enantiomerization of Axially Chiral Biphenyls: Polarizable MD Simulations in Water and Butylmethylether. International Journal of Molecular Sciences, 2020, 21, 6222.	1.8	4
85	The influence of the cation structure on the basicity-related polarity of ionic liquids. Physical Chemistry Chemical Physics, 2021, 23, 26750-26760.	1.3	4
86	Collectivity in ionic liquids: A temperature-dependent, polarizable molecular dynamics study.. Physical Chemistry Chemical Physics, 0, , .	1.3	3
87	Charged, dipolar soft matter systems from a combined microscopicâ€“mesoscopic viewpoint. Journal of Physics Condensed Matter, 2016, 28, 344008.	0.7	2
88	General review of ionic liquids and their properties. , 2016, , 1-23.		1
89	Dielectric spectroscopy and time dependent Stokes shift: two faces of the same coin?. Physical Chemistry Chemical Physics, 2020, 22, 18388-18399.	1.3	1
90	Proteins in Ionic Liquids: Current Status of Experiments and Simulations. , 2017, 375, 1.		1

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91	Computational solvation dynamics: Implementation, application, and validation. Annual Reports in Computational Chemistry, 2020, , 93-154.	0.9	1
92	Grid Services for Parallel Molecular Dynamics with NAMD and CHARMM. Lecture Notes in Computer Science, 2008, , 1036-1051.	1.0	1